Energetic Instability Unjams Sand and Suspension

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Abstract

Jamming is a phenomenon occurring in systems as diverse as traffic, colloidal suspensions and granular materials. A theory on the reversible elastic deformation of jammed states is presented. First, an explicit granular stress-strain relation is derived that captures many relevant features of sand, including especially the Coulomb yield surface and a third-order jamming transition. Then this approach is generalized, and employed to consider jammed magneto- and electro-rheological fluids, again producing results that compare well to experiments and simulations.

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We start our study of jamming [1] in granular systems, by deriving an appropriate stress-strain relation from a simple, postulated elastic energy. It accounts for the reversible elastic deformation of granular systems, up to the point of yield, and reproduces many relevant results from granular physics and soil mechanics [2, 3], including the compliance tensor, *Rankine* states, and shear dilatancy. Moreover, the elastic energy is convex only below the Coulomb yield condition and becomes unstable there. As a result, the system escapes from the strained state and looses shape-rigidity, providing an explanation why sand unjams. Next, the granular elastic energy is shown to be a special case of a more generally valid energy expansion, with respect to the shear strain. Realizing that this expansion may serve as the starting point to account for other jammed systems, we use it to consider colloidal suspensions [4], specifically magneto- and electro-rheological fluids, which solidify at fields strong enough [5, 6]. Again, an energy expression is proposed, from which the magnetic, dielectric and elastic behavior is deduced, especially the solid-fluid phase diagram.

Our basic understanding of sand is due to Coulomb, who noted that its most conspicuous property is yield: A pile of dry sand possesses a critical slope that it will not exceed. His insightful conclusion is that the quotient of shear stress over pressure must not exceed a certain value, $|\sigma_s|/P \leq \mu_f$. Wet sand can sustain a small shear stress σ_c even at vanishing pressure. It satisfies the *Mohr-Coulomb* condition, $|\sigma_s| \leq \mu_f P + \sigma_c$, see [7].

It is standard praxis in soil mechanics to calculate the stress distribution by taking the stress σ_{ij} as some function of the strain u_{ij}. Unfortunately, the calculated stress distribution routinely contradicts the Coulomb condition, and yield must be postulated, *ex post facto*, where it is not satisfied. An improvement of this somewhat brute method is given by the *Rankine* states, $\sigma_s = \pm P\mu_f$, which should hold close to yield. The ameliorated calculation is given by accepting the result of elasticity away from the region of failure, postulating a Rankine state close to it, and connecting both smoothly. Clearly, in spite of ingenious ways to circumvent it, the basic problem is the lack of a stress-strain relation $u_{ij}(\sigma_{kl})$, with which a realistic stress distribution can be calculated.

If we had $u_{ij}(\sigma_{kl})$, the incremental relation, $\delta u_{ij} = (\partial u_{ij}/\partial\sigma_{kl})\delta\sigma_{kl} \equiv \lambda_{ijkl}\delta\sigma_{kl}$, is easily derived. The elements of the compliance tensor λ_{ijkl} can also be obtained from experiments, in which δu_{ij}, the strain response to a stress change $\delta\sigma_{ij}$, is measured [8]. Although integrating the measured λ_{ijkl} should in principle lead to $u_{ij}(\sigma_{kl})$, this is a hard, backward operation – made more difficult by the typical scatter of data, partly from irreversible plastic deforma-

tions. This circumstance has led many to espouse the view that λ_{ijkl} is history-dependent, that an explicit $u_{ij}(\sigma_{kl})$ (from which to deduce λ_{ijkl}) does not exist. Different elasto-plastic theories, some exceedingly complex, have been constructed to account for λ_{ijkl}, including both elastic and plastic deformations, though a universally accepted model is missing [3].

Confining our study to reversible elastic deformations, we derive a stress-strain relation to account for the listed granular behavior. We start from the elastic energy

$$w = \tfrac{1}{2}\delta^{0.5}(B\delta^2 + Au_s^2), \tag{1}$$

where $\delta \equiv -u_{\ell\ell}$ is the compression, $u_s^2 \equiv u_{ij}^0 u_{ij}^0$ is shear strain squared. ($u_{\ell\ell}$ denotes the trace of the strain and u_{ij}^0 its traceless part. $\delta, u_s = 0$ imply the grains are in contact but not compressed or sheared.) $A, B > 0$ are functions of the void ratio e, an independent variable. We adopt the same empirical expression for both, $A, B \sim (2.17 - e)^2/(1 + e)$, see [8]. Eq (1) is clearly evocative of the Hertz contact: The energy of compressing two elastic spheres scales with $(\triangle h)^{2.5}$, where $\triangle h$ is the change in height [9]. Writing the energy as $\frac{1}{2}E(\triangle h)^2$, the effective Young modulus $E \sim (\triangle h)^{0.5}$ vanishes with $\triangle h$. The physics for the shear modulus is assumed to be similar.

We postulate Eq (1) to consider its ramifications – noting that it should be possible to derive it employing micro-mechanics [10]: Although an intricate task, it is not as difficult as calculating the stress σ_{ij} or the compliance tensor λ_{ijkl} directly. Remarkably, assuming that both moduli vanish with $\delta^{0.5}$, we take sand to be arbitrarily pliable, not at all “fragile” [11]. Differentiating the energy w with respect to δ, u_s yields the pressure P and shear σ_s, two scaler quantities; differentiating it with respect to u_{ij} yields the complete stress tensor σ_{ij},

$$P \equiv \partial w/\partial\delta = \tfrac{5}{4}B\,\delta^{1.5} + \tfrac{1}{4}A\,u_s^2/\delta^{0.5}, \tag{2}$$

$$\sigma_s \equiv \partial w/\partial u_s = A\,\delta^{0.5}\,u_s. \tag{3}$$

$$\sigma_{ij} \equiv \partial w/\partial u_{ij} = -P\delta_{ij} + A\delta^{0.5}u_{ij}^0. \tag{4}$$

This is the announced static stress-strain relation. The first term in P is well-known and considered characteristic of Hertz contacts. The second term, accounting both for shear dilatancy and yield, is new. Dilatancy: Holding P constant, δ decreases (and the volume expands) with growing u_s. Yield: For given u_s, the compressibility $(\partial P/\partial\delta)^{-1}$ is negative if δ is sufficiently small. This implies lack of local stability, and the system will not remain in the strained state. It is then, without the capability to sustain static shear, in

a fundamental sense "fluid" – though by no means necessarily Newtonian. In fact, the energy looses stability even before $\partial P/\partial\delta$ turns negative, as the cross convexity condition $(\partial^2 w/\partial\delta^2)(\partial^2 w/\partial u_s^2) \geq (\partial^2 w/\partial\delta\,\partial u_s)^2$, or $u_s^2/\delta^2 \leq 5B/2A$, also needs to be met. We saw the significance of instability in a previous work [12], but did not realize the following remarkable point and its consequences: Rewriting the cross convexity condition by replacing δ, u_s with P, σ_s leads directly to (the *Drucker-Prager* variant [7] of) the Coulomb yield condition,

$$|\sigma_s|/P \leq \sqrt{4A/5B}. \tag{5}$$

To account for wet sand, the term $-P_c\delta$ (with $P_c > 0$) is added to the energy w. This implies a force (typically supplied by the water's surface tension) that compresses the grains even without an applied pressure. The additional term does not change the convexity condition, only substitutes $P + P_c$ for P in Eq (2). As a result, Eq (5) assumes the *Mohr-Coulomb* form, $|\sigma_s| \leq (P + P_c)\sqrt{4A/5B}$.

As any other elasticity theory, the stress-strain relation of Eqs (2,3,4) may be directly solved with appropriate boundary conditions to obtain a complete stress distribution. Because it includes yield as given by Eq (5), the *Rankine* states are automatically predicted where instability is close. And the compliance tensor λ_{ijkl} is obtained by simple differentiation. Writing $\delta u_{ij} = \lambda_{ijkl}\delta\sigma_{kl}$ as a vector equation, $\delta\vec{\sigma} = \hat{M}\delta\vec{u}$, with $\hat{M}$ a 6×6 matrix, we see yield is signified if an Eigenvalue m_1 of $\hat{M}$ vanishes, with the Eigenvector $\delta\vec{u}_1$ indicating the direction of instability. Explicit calculation shows $\delta\vec{u}_1 \| (\partial m_1/\partial\vec{\sigma})$, implying $\delta\vec{u}_1$ is perpendicular to the yield surface, $m_1(\vec{\sigma}) \sim |\sigma_s| - P\sqrt{4A/5B} = 0$. If there is no plastic contribution, this implies flows perpendicular to the yield surface, a circumstance referred to as the "associated flow rule" [7].

In view of these results, there can be little doubt that Eq (1) indeed captures the essence of granular elasticity. And the remaining question is: To which extent is it also a quantitative rendition. To test this, we compare the calculated λ_{ijkl} to the data gathered recently [8], over a wide range of pressure, shear stress and void ratio. (Specifying these three variables, the reversible granular response is unique, showing no history-dependence.) Fig. 1 is a typical plot, with an overall agreement that further confirms Eq (1). (The expression for λ_{ijkl} is too cumbersome to be displayed here. It will be given in a forthcoming single-issue paper containing extensive comparison.) Note the ratio A/B is fixed by the Coulomb friction coefficient μ_f, so the theory has only one overall scale factor, and no actual adjustable

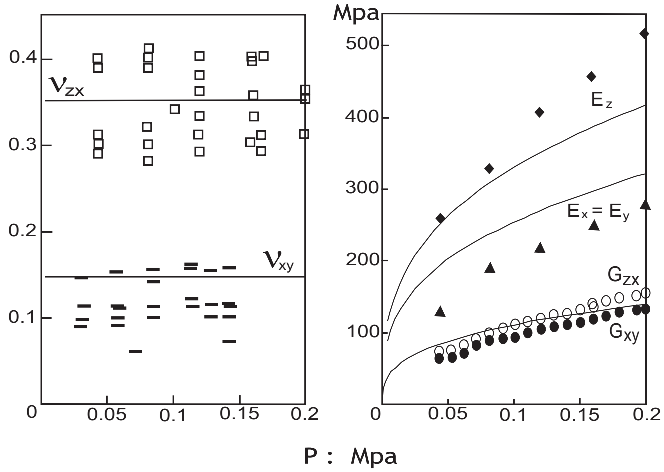

FIG. 1: The Poisson ratios ν_{zx}, ν_{xy}, the Young moduli $E_z, E_x = E_y$, and the shear moduli G_{zx}, G_{xy}, measured [8] with Ham River sand at $\sigma_{xx}/\sigma_{zz} = 0.45$ and a void ratio of 0.66, compared to the calculated curves assuming $B = \frac{2}{3}A = 6800$Mpa, with $E_i \equiv \lambda_{iiii}^{-1}$, $G_{ij} \equiv \frac{1}{2}\lambda_{ijij}^{-1}$, $\nu_{ij} \equiv -\lambda_{iijj}/\lambda_{iiii}$. ($x$, y are horizontal directions, z the vertical one.) Note these coefficients are pairwise equal for linear elasticity, but deviate from each other nonlinearly; theory and experiment especially agree with respect to the direction of deviations, ie., the fact that $\nu_{zx} > \nu_{xy}$, $E_z > E_x = E_y$, $G_{zx} = G_{xy}$.

parameter. (The most important effect missing in Eq (1) is probably "fabric-anisotropy" [2].)

Switching now to a broader context, we proceed to discriminate between the general feature of the above theory and those aspects specific to granular elasticity. This should give us a better appreciation why Eq (1) is as successful, and also help to apply the same approach to other jammed systems. Generally speaking, the energy should be a function of at least two variables, u_s and f, with f being the one driving the transition, taking place at f_c. In sand, suspensions, and electro-rheological fluids, f is respectively given by the compression δ, concentration, and the electric field. Expanding the energy in u_s,

$$w = w_0(f) + \tfrac{1}{2}Ku_s^2, \tag{6}$$

the shear modulus K is a function of f, typically $K \sim (f - f_c)^a$ with $a > 0$ in the solid phase ($f > f_c$), and $K \equiv 0$ in the liquid one ($f < f_c$). This dependence is observed in suspensions [4], simulations [14] and, with $a \approx \frac{1}{2}$, works well for sand. We take it as an input. Local stability requires $K > 0$ and

$$w_0'' > [(K')^2/K - \tfrac{1}{2}K'']u_s^2 \equiv \kappa u_s^2, \tag{7}$$

ensuring w is convex in f, u_s. Because $\kappa \sim a(a+1) \times (f_c - f)^{a-2}$ is positive, the inequality is always violated when u_s becomes sufficiently large, rendering instability, and hence the unjamming transition, a generic feature. If $a < 2$, κ diverges for $f \to f_c$, and unjamming occurs at vanishing values of u_s (assuming w_0'' remains finite). This ensures the validity of the expansion of Eq (6).

Considering the jamming transition in the shear-free limit $u_s \to 0$, we identify it – by analogy to conventional phase transitions – as of n^{th} order, if $\partial^i w_0/\partial f^i$ is continuous for $i < n$, but not for $i = n$. With $w_0 \sim \delta^{2.5}$, sand displays a third-order jamming transition.

Yield at finite shear, as a result of the energetic instability, Eq (7), is not an equilibrium transition, because the liquid phase moves and dissipates. This may well be compared to raising the temperature T in a current-carrying superconductor, such that the metal is pushed into its normal state carrying a dissipative, ohmic current. In fact, if one identifies f as T, replaces u_s with the superfluid velocity v_s (and hence σ_s with the current, $j_s = \rho_s v_s$), Eq (6) is valid for superconductors, and superfluid helium, $\frac{1}{2}K u_s^2 \to \frac{1}{2}\rho_s v_s^2$, respectively with $\rho_s \sim T_c - T$ and $\rho_s \sim (T_c - T)^{2/3}$ [15]. Macroscopically, jamming and phase transition are clearly hard to tell apart, and their conceptual difference must be subtle.

Next, we consider ER and MR (or electro- and magneto-rheological) fluids, employing them as further examples for the above notion of jamming. Although experimental data are as yet not confining enough for an unambiguous determination of their energy, plausibility may be drawn on to fill the gap. In ER fluids, the dielectric displacement D assumes the role of the transition-driving variable f. Writing the shear-free part of the energy as $w_0 = w_1 + w_2$, we take $w_1 = \frac{1}{2}D^2/\epsilon_1$, accounting for a linear dielectric relation, and $w_2 = -\frac{1}{2}\triangle(D - D_c)^2$, assuming that linearity prevails after the transition at D_c. This is a second-order transition, and the electric field $E \equiv \partial w/\partial D$ has a kink at D_c: We have $E = D/\epsilon_1$ for $D \leq D_c$, and $E - E_c = (D - D_c)/\epsilon_2$ for $D > D_c$, with $1/\epsilon_2 = 1/\epsilon_1 - \triangle$, $E_c \equiv D_c/\epsilon_1$. (A discontinuity in E, or a first-order transition, was to our knowledge never reported. Higher order transitions are possible, seem even likely, but they are not compatible with a linear constitutive relation after the transition.) w_2 is the condensation energy, so $\triangle$ must be positive for solidification to take place. (Taking $D \to B$, $E \to H$ yields the analogous formulas for MR fluids.) Given w_0 and $K = A(D - D_c)^a$, the energy w of Eq (6) is specified. We calculate the dielectric relation $E \equiv \partial w/\partial D|_{u_s}$, elastic relation $\sigma_s \equiv \partial w/\partial u_s|_D$, and rewrite Eq (7) in terms of E, σ_s

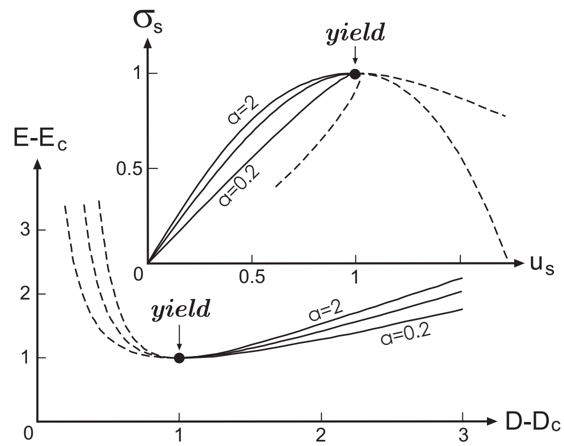

FIG. 2: Elastic and dielectric properties, including the yield point, for electro- and magneto-rheological fluids: Shear stress σ_s versus shear strain u_s at fixed electric field E, and $E-E_c$ versus $D-D_c$ (or $H-H_c$ versus $B-B_c$) at fixed σ_s, for the exponents $a=2,1,0.2$. Choosing the dimension of both curves such that the yield points are at (1,1) render the curves universal – removing the dependency on (i) all material parameters other than the exponent a, (ii) E in the upper plot, and (iii) σ_s in the lower one. The relation $\sigma_s(u_s)$ for $a=1,2$ agree with data from experiments and simulations [18].

to obtain the yield condition,

$$|\sigma_s| \leq (E-E_c)^{1+\frac{a}{2}}\sqrt{2A\frac{[\epsilon_2(a+1)]^{a+1}}{a(a+2)^{a+2}}}. \tag{8}$$

The exponent $a=1$, or a yield stress $|\sigma_s| \sim (H-H_c)^{3/2}$ is observed for most MR-fluids [16]. The same value is also appropriate for a few ER-fluids [17], though the yield stress is typically quadratic [5, 18], $|\sigma_s| \sim (E-E_c)^2$, indicating $a=2$. An ER-fluid capable of sustaining an unusually high shear strength was reported [6] to display a nearly linear dependence of the yield stress, $|\sigma_s| \sim E-E_c$, or $a \ll 1$. For $a=0$, the shear modulus K is independent of the field, and there is no yield at all. This is the reason the square root in Eq (8) diverges for $a \to 0$, and possibly explains the observed high yield stress.

Finally, the above approach and results are critically appraised. (Granular vocabulary is employed for this purpose, though the statements are equally valid for ER and MR fluids.) In physics, every microscopic state has a unique energy. The same holds for macroscopic ones if we insist on a consistent description. The macroscopic energy always depends on entropy

and conserved quantities, such as momentum and mass density. And if the considered system can sustain static shear stresses, the strain field u_{ij} must also be included as an independent variable, where u_{ij} is to be understood, in soil-mechanical parlance, as the reversible elastic portion of the strain field.

It is a plain fact that sand piles, if left alone under gravity, are stable – in spite of every kind of infinitesimal perturbations, which are always present. This demonstrates sand's capability to sustain static shear and is the reason for including u_{ij}. Irrespective whether a unique displacement field exists, the elastic description employing u_{ij} is robust enough to be valid. This is not different from superfluid helium with vortex lines, in which the description in terms of the velocity $\boldsymbol{v}_s = \frac{\hbar}{m}\boldsymbol{\nabla}\phi$ remains sound, although the phase field ϕ is multivalued.

Given an energy expression w, its derivative $\partial w/\partial u_{ij}$ yields the stress tensor σ_{ij}, and its second derivative $\partial^2 w/\partial u_{ij}\partial u_{kl}$ the inverse of the compliance tensor λ_{ijkl}. In soil mechanics, the usual approach consists of postulating the stress dependence of the 18 independent components of λ_{ijkl} directly, while seeking the account for the plastic contribution at the same time, referring to the result as constitutive relations [3]. This is quite obviously a much harder task than finding the one appropriate scalar expression for the energy w which, even if heavy-handedly simplified, preserves a large number of geometric correlation by the mere fact that λ_{ijkl} is obtained via a double differentiation. We believe this to be the main reason why the calculated λ_{ijkl} stood up so well when compared to the extensive data of [8].

The expression we proposed in Eq (1) is indeed the result of weighing simplicity versus accuracy while stressing the former, and hence is subject to further scrutiny. As discussed, it includes first of all an expansion in u_s: $w = \frac{1}{2}Ku_s^2$ assuming $K \sim \delta^a$. Starting from $w = \frac{1}{2}(B\delta^{2+b} + A\delta^a u_s^2)$ in [12], we considered the experiments of inclined plane, simple shear and triaxial test to arrive at $a \approx 0.4$, $b \approx 0.5$ giving the best agreement [19]. On the other hand is the fact that the Coulomb yield condition, Eq (5), remains unchanged as long as $a = b$. And it becomes implicit if a, b deviate from each other – though the numerical difference is at first modest. Our tentative choice is $a = b = \frac{1}{2}$.

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